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# Attended Lectures in Other Fields, as a Participating Guest in the Detonator and Detonation Physics Group

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## **ATTENDED LECTURES IN OTHER FIELDS, AS A PARTICIPATING GUEST IN THE DETONATOR AND DETONATION PHYSICS GROUP**

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### **1.1 INERTIAL CONFINEMENT FUSION ABLATOR APPLICATION**

- CMS Post Doc Brown Bag Seminar "Characterization and Mechanical Behavior of Nanoporous Metal Foams" by Andrea Hodge, Nanoscale Synthesis and Characterization Laboratory, Materials Science and Technology Division

- CMS Post Doc Brown Bag Seminar, "Diamond Ablators for Inertial Confinement Fusion" by Juergen Biener, Nanoscale Synthesis and Characterization Laboratory, Materials Science & Technology Division : Diamond has a unique combination of physical properties for the inertial confinement fusion ablator application, such as appropriate optical properties, high atomic density, high yield strength, and high thermal conductivity. I will report on some of the recent progress made in the fabrication of diamond ablator shells.

### **1.2 NUCLEAR SCIENCE**

- Physics and Advanced Technologies, I-Div/Radiation Detection Center Seminar, Dr. Mark Wallace, Post-Doctoral Applicant, Michigan State University : Experimental and Theoretical Challenges in understanding the rp-process on accreting neutron stars. The rp-process is responsible for observed X-ray bursts originating from accreting neutron stars in binary systems. This explosive process drives nucleosynthesis toward the proton drip line where little experimental data exists, making it necessary to rely on models. In the context of a specific rp-process model, the relevance of mass measurements for proton rich nuclei will be discussed. An experimental technique, based on the study of (p,d) reactions, will be presented. This technique provides a powerful tool to determine the mass of proton rich nuclei with high accuracy. For this purpose, high-resolution detectors have been developed. The performances of such devices and the current experimental program will be discussed.

- NUCLEAR SCIENCE, SCIENCE INTERNSHIP PROGRAM SEMINAR, Forensic Radiochemistry, Ken Moody, Chemical Biology and Nuclear Science Division, LLNL

- NUCLEAR SCIENCE SCIENCE INTERNSHIP PROGRAM SEMINAR, Atom-at-a-Time Studies of the Transactinides, Darleane Hoffman, Prof. of the Graduate School, Dept. of Chemistry, UC Berkeley & Faculty Sr. Scientist, Nuclear Science Division, Lawrence Berkeley National Laboratory

- Phonon density of state in Pu, Dr Joe Wong

### **1.3 CRYSTAL DEFECTS**

- Chemistry and Materials Science and Polytechnic University of Madrid, Spain, M.Victoria, Are metallic nanocrystals radiation resistant ?

- Royal Institute of Technology, Sweden, Göran Grimvall : How Superheated Crystals Melt

In experiments where intense radiation penetrates into the bulk of a solid and causes ultrafast (femtosecond) heating, the superheated crystalline solid melts from within at a temperature above the equilibrium melting temperature. But what happens on the atomic scale as a solid loses crystalline order remains an open question. Molecular dynamics modeling allows the position of every atom to be traced at each instant, as a crystal transforms from solid to liquid. Here we use such detailed atomistic simulations, relevant for aluminum, to show that the thermal fluctuation initiating melting is an aggregate typically with 6-7 interstitials and 3-4 vacancies. This mechanism differs from those that have traditionally been proposed, which generally involve many more atoms at the initial melting stage.

- Dr Belak, Use of synchrotron to characterize dynamically the defects, cracks formation in Aluminum and metals induced by a slapper

- G.Overturf, Study of TATB ratchet growth using SAXS

- CMS Post Doctoral Symposium, Raluca Negres, Behaviour of Initiating Defects in KDP and DKDP Crystals Under Laser Irradiation

- 3 omega damage in fused silica, Dr Joe Wong

### **1.4 PHASE TRANSITION**

- Livermore Computing / Computation, Nir Goldman, Chemistry and Materials Science Directorate, Simulations of Water in Giant Planets : Discovery of Symmetric H-Bonding in the Superionic Phase.

- Chemistry and Chemical Engineering Division Energetic Materials Center – Extreme Chemistry, Stefanie Japel, Postdoctoral applicant, The Johns Hopkins University and Carnegie Institution of Washington Geophysical laboratory, Diamond-anvil cell high-pressure high temperature experiments : Applications in earth science and beyond.

- CMS Post Doctoral Symposium, Thaddeus Norman, The transmission spectrum of DKDP in a Diamond Anvil Cell

- Chemistry and Chemical Engineering Division, Energetic Materials Center - Extreme Chemistry, Postdoc Applicant Seminar, Dr. Zhongwu Wang, Los Alamos National Laboratory : Exploring the size- and morphology -induced mechanism in nanomaterials under extreme conditions

Mechanical properties and phase transformation of materials depend significantly on the size of the crystalline grains. Upon decrease of particle size to nanometer, materials exhibit either novel, enhanced or weakened properties compared to their bulk counterparts. The increased surface energy tuned by small particle size results in a structural instability of materials, whereas the surface reconstruction with specific low-energy crystallographic facets leads to the enhanced stability of materials. Therefore, the effects induced by the size and specific morphology compete each other and cast a significant impact on the extended properties of nanomaterials. With rapid development of high-pressure techniques, the pressure tuning is certainly the most simple and feasible tool that allows one to directly observe and study the size- and morphology induced phenomena and resulting mechanism. I have performed the detailed high pressure studies with different experimental designs on three types of nanomaterials, including hard materials (single crystal and composites), semiconductors (one, two and three dimensional nanocrystals) and carbon forms. I will briefly highlight the feasible high pressure techniques, present the preliminary experimental results with focuses on elastic modulus, transformation, nucleation, growth and fracture, yield strength and hardness, and further discuss the resulting mechanism with close relation to surface energy and its crystallographic dependence, critical size, and interface action.

## **1.5 BINDER**

- CMS Post Doc Brown Bag Seminar, "Novel synthetic methodologies and materials in the advanced materials synthesis group" by Brady Clapsaddle, Advanced Materials Synthesis Group, Chemical and Chemical Engineering Division, The talk will discuss recent advances in our group in the area of sol-gel chemistry and materials preparation. Synthesis of nano-particles, scintillators, and ceramic materials, to name a few, will be discussed.

- CMS Post Doc Brown Bag Seminar, "Molecular Dynamics Simulations of Ordering in Polymers" by Naida Lacevic, XChem, Chemical and Chemical Engineering Division:

Large scale molecular dynamics simulations of bulk melts of polyethylene (PE), poly(vinylidene fluoride) (pVDF), and poly(dimethylsiloxane) (PDMS) are utilized to study chain conformation and ordering prior to crystallization under cooling (PE and pVDF) or uniaxial extension (PDMS). Some recent results on spinodal-assisted crystallization of PE and pVDF under deep quench as well as ordering and cavitation of PDMS will be discussed.

- Chemical Biology & Nuclear Science Division, Chemistry & Materials Science Directorate, Seth Gleiman, Materials Team, Materials and Explosives Engineering Group, Engineering, Sciences and Applications Division, Los Alamos National Laboratory, "Environmental Effects on LK3626 Flat Slab Load Response (U)" (Foreign Nationals may attend if appropriate security plan is on file, which includes B-151) : LK3626 is a hydrogen-blown, RTV silicone foam catalyzed by stannous octoate, a tin compound with complex chemistry. The active form of the catalyst requires it to be reversibly hydrated so that a tin hydroxide is formed, along with the resulting octanoic acid byproduct. Postcure of the foam is supposed to eliminate the activity of the catalyst thereby stopping any additional reaction from occurring. Yet, it is believed that postcuring does not deactivate the catalyst. Rather, as parts sit on the shelf awaiting qualification they may absorb ambient moisture and reactivate the catalyst thereby causing additional reaction indicated by incremental stresses developed at any strain. This work is meant to examine the effect of storage condition, specifically relative humidity, on the load response of LK3626 as a function of storage time. While a stress enhancement was not observed for any environmental condition up to 10 days, interesting results are presented that provide insight to the action of the catalyst and the filler effect during the rest period after manufacture prior to postcure. Results are presented that compare mechanisms for samples stored in dessicated environments to samples that are stored under ambient conditions and then postcured.

- Chemical Biology & Nuclear Science Division, Chemistry & Materials Science Directorate, Seth Gleiman, Materials Team, Materials and Explosives Engineering Group, Engineering, Sciences and Applications Division, Los Alamos National Laboratory, "Predicting Polymer Molecular Weight Distribution and Network Topology in Silicone Networks (U)" : Several theories exist for the description of network topology in crosslinking systems. A short background of the Miller/Macosko theory, based on the recursive nature of crosslinking systems, is presented with examples. This theory is applied to network-forming materials of interest to the Materials Team. The results for simple, two-component systems are presented along with first approximation results for a complex reacting system with multiple reactants and functionalities. Experiments to validate the model will be presented and limitations of the model will be discussed. Future work to increase model complexity will be outlined.

- Chemistry and Materials Science Directorate, MATERIALS SCIENCE AND TECHNOLOGY DIVISION, JAMES E. SHEPHERD (Postdoc applicant) (US Citizen) GEORGIA INSTITUTE OF TECHNOLOGY ATLANTA, GEORGIA, Multi-scale modeling of the Deformation of Semi-Crystalline Polymers : The mechanical and physical properties of polymers are determined primarily by the underlying nano-scale structures such as entanglements, crystallites, and molecular orientation. These structures

evolve during the processing of polymers into useful articles. Limitations of available and foreseeable computational capabilities prevent the direct determination of macroscopic properties directly from atomistic computations of the nano-scale structures. As a result, computational tools and methods to bridge the length and time scale gaps between atomistic and continuum models are required. An internal state variable continuum model has been developed whose state variables and evolution equations are related to the nano-scale structures. In this research, separate atomistic models and methods have been developed to investigate the primary nano-scale structures that affect mechanical behavior, the evolution of entanglements, crystallization, and other molecular interactions during thermo-mechanical deformations. The results of these simulations are used to gain a clearer understanding of the mechanisms involved to enhance the physical basis of the evolution equations in the continuum model and to derive the model's material parameters. The end result is a continuum model that reflects the atomistic structure of the polymer. Ideally, the methods employed will be general enough to be applicable to most types of polymer systems.

## **1.6 BIOSENSING**

- Biosciences directorate seminar series, Microbial iron oxidation at neutral PH : biofilms and biomineralization, Dr Clara Chan, Banfield Geomicrobiology group, Dept. Of Earth and Planetary Science, University of California, Berkeley

- Chemistry & Materials Science Directorate (CMS), Chemical Biology & Nuclear Science Division (CBND), Postdoc Applicant Seminar, Nicole Chakov, University of Florida, Gainesville, "MOLECULAR MANGANESE COMPOUNDS AS SINGLE-MOLECULE MAGNETS: A MOLECULAR APPROACH TO NANOSCALE MAGNETS"

Single-molecule magnets (SMMs), or molecules that function as single-domain magnetic particles, represent a molecular approach to nanoscale magnetic materials. They exhibit slow magnetization relaxation at low temperatures, resulting in hysteresis loops, the classical property of a magnet. Due to their nanoscale dimensions, SMMs represent the point at which classical and quantum worlds meet, being mesoscopic entities which display quantum effects. Such molecules have potential applications for high density information storage at the molecular level as well as qubits in quantum computers. The latter is a consequence of their ability to undergo quantum tunneling of magnetization (QTM). The most well-studied SMMs with the highest energy barriers to magnetization relaxation are members of the  $[\text{Mn}_{12}\text{O}_{12}(\text{O}_2\text{CR})_{16}(\text{H}_2\text{O})_4]$  family. Modifications to the Mn<sub>12</sub> complexes, including the use of non-carboxylate or bulky, hydrophobic ligands and changes to the oxidation level, have been introduced to probe their influence on the above-mentioned properties. Such studies are quintessential for a complete understanding of the structural factors that influence the magnetic behavior of SMMs and are described herein.

- Chemical Biology and Nuclear Science / Biosecurity and Nanosciences Laboratory, Amy Gryshuk, Suny at Buffalo, Photodynamic Therapy Photosensitizers for Cancer Treatment and Diagnosis.

- BIOSCIENCES DIRECTORATE SEMINAR SERIES, "Translational technology to Mix and Match 100 things!", Dr. Kodumudi "Venkat" Venkateswaran, Biodefense Division

## **1.7 NANOTECHNOLOGY**

- Chemistry and Materials Science Frontiers Symposium, Paul Alvisatos, UC Berkeley, Colloidal Nanocrystals : Synthesis, Properties, Applications.

Over the last decade there have been significant advances in the ability to prepare colloidal inorganic nanocrystals with controlled size, shape, and even interconnection (branching) and topology (hollow and nested). These materials exhibit strongly size dependent properties, but they also share many of the characteristics of inorganic solids, in terms of stability and range of properties. They can be processed in solution like polymers. They thus make attractive candidates for incorporation into a range of technologies, from biological labels to components in solar cells and catalysts.

- Chemical Biology and Nuclear Science / Biosecurity and Nanosciences Laboratory, Soojin Oh, postdoctoral applicant, University of North Carolina, Assembly and Integration of Functional Carbon Nanotube Structures.

- Materials Science & Technology Division, Seminar Announcement, "Surface Chemistry at the Nanoscale", Fernando Reboredo, H-Division :

When the size of a material is reduced to nanometers, a significant fraction of the atoms (25-50 %) is directly at the surface. Therefore, the relevance of the surface on the properties of the cluster increases. Conventional wisdom suggests that chemical properties are highly local, depending mostly on atoms at short distances. According to that wisdom, the chemistry of nano-structured elements should not be very different from the chemistry of the same elements in bulk form. Although in general that line of thought is correct, there are several exceptions: i) Quantum confinement changes the optical properties of nanomaterials; these changes, in turn, can have a strong impact on reactions catalyzed by light. ii) Several metals in bulk form act as catalyst of important chemical reactions. Conventional wisdom would suggest that they would be better catalyst at the nanoscale than in the bulk, because of a larger surface to volume ratio. However, when the size of a catalyst is reduced to the nanoscale, the electronic properties change. A change in electronic properties should have an impact on chemical properties. Therefore, whether a given element is a better or worse catalyst at the nanoscale than in bulk form, remains an open question. iii) Conversely, surface chemistry has a strong impact on the properties of nanomaterials (since a significant fraction of the atoms are at the surface) which in turn has a feedback effect both in physical and chemical properties. In this talk we will discuss several examples of nano-scale-induced changes in chemistry for semiconductor and metallic nanocrystals. In particular we will discuss examples in Si, SiC and Cobalt nanoclusters.

- Chemical Biology and Nuclear Science Directorate, Biosecurity & Nanosciences Laboratory, Post Doctoral Applicant Seminar, Dr. Nitin Chopra, University of Kentucky at Lexington : "Selective Growth of 1-D Nanostructures: Applications in Shadow Lithography and Aligned Carbon Nanotube Membranes"

Due to their micron-scale length, nanotubes and nanowires can be manipulated with current microfabrication techniques yet result in nm-scale features inherent to their diameter. A promising approach investigated here is to utilize thin film multilayer structures where the thickness of a catalyst layer at an exposed edge of photolithographically defined pattern determines the diameter of nanotubes/nanowires grown from it. This can in turn be incorporated into photolithographically defined "post" structures resulting in an array of suspended nanowires for line-of-site shadow lithography. In principle this would result in a high throughput nm-scale lithography process based on conventional lithography process and nanowire growth. Success of the diameter control approach has been shown by selectively growing carbon nanotubes (CNTs) from narrow lines (12-60 nm) of SiO<sub>2</sub>, Fe, Ni, Co on micron-scale patterned substrates in a ferrocene or non-ferrocene catalyzed CVD process. In addition, the concept has been extended to VS growth of CuO nanowires and VLS growth of ZnO nanowires from an exposed edge in an Al<sub>2</sub>O<sub>3</sub>/Cu (40-100 nm)/Al<sub>2</sub>O<sub>3</sub> and Al<sub>2</sub>O<sub>3</sub>/Au (10 nm)/Al<sub>2</sub>O<sub>3</sub> thin film multilayer structures. The exposed middle layer of patterned thin-film multilayer acts as a nm-scale wide selective growth area. As confirmed by TEM and SEM, the resultant CNT/nanowire diameter is directly related to catalyst/catalyst support size. Growth kinetic Studies of CuO nanowires from a thin film multilayer structure indicate a diffusion-controlled process.

Dispersion of CNTs or thermal growth of CuO nanowires between lithographically defined trenches of width of 200 nm and depth of 500 nm when coupled with line-of-site deposition resulted in nm-scale line underneath the suspended nanostructures. The width of the resulting shadow is nearly a simple function of CNT/nanowire diameter, incident evaporation angle, and height of CNT/nanowire above the substrate in a line-of-site evaporation geometry. However by careful analysis in a direct measurement of CNT diameter and shadow width, it was found that shadow width deviates by as much as 7nm at incident angles of 2 degrees. Another promising approach to control the placement of nanotubes/nanowires is the selective functionalization of only their tips followed by self-assembly onto chemically patterned substrates. Towards this goal, arrays of aligned CNTs were impregnated with polystyrene to form aligned CNT membranes. These CNT membranes were characterized by TEM, SEM, gas and ionic transport studies. Different functionalization chemistry was performed on each side of the membrane. After dissolution of polymer matrix, a suspension of CNTs with different functionality at each tip was formed, allowing for sophisticated self-assembled architectures. Such functionalization methodology is also important for studies related to molecular-scale controlled flow or separations using aligned CNT membranes with applications in biosensing.

- Chemical Biology and Nuclear Science Division, Biosecurity & Nanosciences Laboratory, Invited Guest Seminar, Dr. Olgica Bakajin, Molecular Biophysics &

## Functional Nanostructures Group : Micro-& Nano-fluids with Proteins and Carbon Nanotubes

In the first part of the talk I will discuss the measurements of kinetics of protein folding at previously inaccessible time scales that have been enabled by the development of microfluidic mixers. We can achieve the fastest mixing time reported while reducing the sample consumption to femtomoles. In addition, in a single experiment, we can observe protein folding on time scales from under 10 microseconds to over 100 milliseconds. Our fastest experimental measurements are now approaching the longest time scales achievable through simulations on LLNL's fastest computers. Our first studies of the fast collapse in a variety of proteins indicate that the collapse may be the rule rather than the exception in the folding process of small proteins.

The other part of my talk will be about the use of carbon nanotubes in applications that range from filters for microfluidic devices and micro-separation and concentration columns, to platforms for studies of nanofluidics, and go as far as nano-scale sensors. I will focus on a project in which we are embedding ordered carbon nanotubes in a thin film to make a semi-permeable membrane with ideal pores. With this architecture we are studying the effects of spatial confinement on molecular transport. Creation of chemically selective membranes with pore diameters commensurable with the size of macromolecules may find practical applications in gas separations, fabrics for protection against CW agents, water demineralization and desalination.

### **1.8 MECHANICAL AND THERMAL PROPERTIES**

- Speaker - Bruce Cunningham, Topic - HE Mechanical Properties Test Activities - An Overview
- Speaker Kevin Vandersall, Run distance to detonation affected by thermal conditions

### **1.9 METROLOGY**

- The ABC of X-ray Absorption Fine Structure (XAFS) Spectroscopy : A Tribute to Dale Sayers – A Modern EXAFS Pioneer, Dr Joe Wong
- Heterodyn velocimeter, T.Whithworth